On Computation of Thermophysical Properties of Pure Gases and Gas Mixtures at High Pressure and Temperature with Chemical Workbench

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Information about thermophysical properties (sound velocity, viscosity, heat conductivity, thermal capacity, etc.) of pure gases and gas mixtures at high pressure and temperature is often necessary in various fields of science and engineering. Data of this kind are available only for technically important gases and are absent for most gases and their mixtures. Even if they were known, it is practically impossible to tabulate such a large amount of information. The only practical way to obtain the necessary thermophysical properties is computation. Reliable methods intended for estimation of the main thermophysical properties of pure gases and their mixtures currently exist. To use these methods, it is necessary to have information about thermodynamic properties of gases, critical parameters and parameters of the model intermolecular potential. Reliable data on thermodynamic properties are available for many gases. However, data on critical parameters and the parameters of intermolecular potential is relatively small.

An attempt was made to develop a database intended for the support of the calculation of thermodynamic properties of pure gases and gas mixtures. The data for thermodynamic properties, critical parameters and parameters of the model intermolecular potential were collected from various data sources. The missing data for some gases were estimated using existing correlations. The software (Chemical Workbench) allows the use of information from the database for computation of such parameters as isobaric and isochoric heat capacities, entropy, enthalpy, sound velocity, adiabatic exponent, viscosity, thermal conductivity, etc.

To compute thermophysical properties of gases and their mixtures at high pressures, we used two real gas equations of state – a virial one with three coefficients, and an equation of state proposed by V.I. Nedostup. The well-known Leonard Jones and Stockmayer potentials were used for intermolecular potentials.

Our investigations have demonstrated that computed values of the thermophysical properties of many gases are in good agreement with tabulated data.